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A preliminary study on applicability of artificial neural network for optimized reflector designs

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Abstract

The neutron reflector is a material to reflect neutrons into reactor cores. The reflectors are designed with their one purpose such as increasing the criticality, specific flux distribution, and others. Generally, the reflector design has been conducted by the experiences of designers due to the lots of design variables such as material selection and arrangement. In this study, the applicability of the artificial neural network is preliminarily studied for the optimization of the reflector arrangement. For the research, a system of artificial neural network was developed using C++ program language. The feedforward neural network was used with three layers which are input, hidden, and output layers. The back-propagation algorithm was adopted for the training of the neural network. After the construction of the neural network system, the optimization and auto machine learning algorithms was developed by C++ programing language for the preliminary study on the applicability of artificial neural network into the reflector design. The results show that the reflector gives a good performance to obtain the goal responses. It is expected that this system can contribute to dramatically increase the efficiency of the reflector designs.

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Keywords: *Artificial Neural Network; ANN, Reflector Design;Fuel Pattern; Arrangement, Optimization; Nuclear Reactor; Criticality;*

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1. Introduction

Reflector is a material which is used for reflecting neutrons generated from the fission reaction of nuclear reactor core. The reflector is used for increasing the efficiency of neutron utilization for the fission chain reactions in reactor core. The graphite, beryllium, steel, water and the others can be used as the reflectors with their one purpose. In research reactors, the various reflectors can be selected and used for their experiment purposes. The reflectors are conventionally designed and arranged by depending on the experiences of the designers. These empirical approaches can cause efficiency problems because it is required to perform lots of estimation trials on their proposed designs and arrangements based on the human experiences. To replace these kinds of human works, artificial neural networks (ANN) has been attention during last decades for lots of fields. The ANN is a virtual algorism developed by imitating human brain neural. The ANN has strength on that it can deduce the prompt answer from arbitrary input, and automatically increase accuracy without any mathematical foundations.

In 1943, a basic idea of the ANN was proposed by Warren McCulloch [1]. They defined the artificial neurons and a cell model with the concepts of weight and activation function. To learn a simple ANN, Frank Rosenblatt introduced a perceptron in 1958 [2]. Using the perceptron theory, the weight, which has a function of brain memory in ANN, is trained and for linear separable problems. The single-layer neural network had a limitation to solve non-linear problems. In addition, lots of transport problems are generally non-linear problems. Therefore, an advanced method should be used for the transport analyses. It was verified that these non-linear problems can be solved with multilayer neural network and backpropagation model. The multilayer neural network is a neural network having more than one hidden layer called feedforward neural network. Generally, this neural network has input layer, hidden layers and output layer. One hidden layer can express all continuous functions and two or more hidden layers can express the non-continuous functions. For the machine learning of the neural network, more than 100 methods are known. The most popular method is the backpropagation method proposed by Bryson and Ho [3]. After those of researches, a lot of methods have been developed to increase the efficiency of the machine learning and accuracy of the neural network.

For the nuclear research field, the application of neural network theory is in a beginning step, and some researches related to the ANN have been notified. In the previous studies, the ANNs are used for the PWR design of core reloading pattern [4-6]. The applications of ANN in these reactors have been used focusing on the loading pattern and design parameters of nuclear reactors. These are generally applied for fixed core configurations, and it can be easily analyzed with the small number of core variables. Also, it has some limitation because the NAA was just used for the data analysis. In cases of research reactors, the core configurations and arrangement including the reflectors and moderators can be significantly changed with their purposes. Due to the core configurations, it has been required lots of the human efforts on its design.

In this study, the applicability of ANN for the design of research reactor core focusing on the reflector arrangement is studied. First, a multilayer neural network was programed with C++ programing language. Using the ANN program, an automatic machine training algorithm was also developed for the reflector designs with MCNP6 code.

2. Method

2.1. Overview of feedforward neural network and back-propagation algorithm

The flowchart of the feedforward neural network used for this study is given in Fig.1. k_{eff} is set to the goal output for the possibility study of the ANN. There are three layers which are input, hidden and output layers. When a material selected from m candidate materials in each region is decided as an initial condition, the input neurons, which is matched to the material number of the region in input layer, is set to 1. At the same time, the other input neurons linked with the region is set to 0. The input signals are linked to the other neurons with weights. For the estimation with the ANN, first, the weighted input is calculated with Eq. (1).

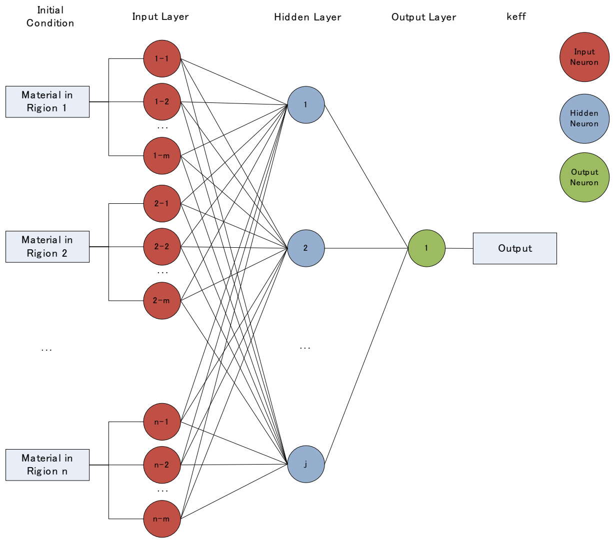


Fig. 1. Overview of feedforward neural network used in this study

$$X_j = \sum_{i=1}^{m\times n} x_i w_{i\to j} - \theta_j \tag{1}$$

where X_j is the weighted input for j^{th} neuron, x_i is the input signal of i^{th} neuron, $w_{i\to j}$ is the weight linked from i^{th} neuron to j^{th} neuron, and θ_j is the threshold value in j^{th} neuron. The output $Y_j^{sigmoid}$ of the j^{th} neuron is calculated by sigmoid activation function as follows:

$$y_j = \frac{1}{1+e^{-X_j}} \tag{2}$$

Among the neurons, the outputs of neurons are estimated with Eqs. (1) and (2) when the input neurons are activated. To obtain an accurate output with the ANN, the $w_{i\to j}$ and θ_j should be accurately estimated and determined from the machine learning. The back-propagation algorithm is generally used for the machine learning [3]. From the big data including inputs and outputs, the back-propagation can be repeated with p times. At each p^{th} repeated step, the error signal of the output for updating the weights and threshold value is calculated defined as follows:

$$E_k(p) = y_{d,k}(p) - y_k(p) \tag{3}$$

where $E_k(p)$ is the error signal at k^{th} neuron at p repetition calculation, $y_{d,k}(p)$ is the goal output of k^{th} neuron at p^{th} repetition and $y_k(p)$ is the output at k^{th} neuron estimated by the ANN at p repetition calculation (result from Eq. (2)). With the error signal, the weight from j^{th} neuron to k^{th} neuron is updated with the weight correction factor $\Delta w_{jk}(p)$ as follows:

$$w_{jk}(p+1) = w_{jk}(p) + \Delta w_{jk}(p) \tag{4}$$

The weight correction factor $\Delta w_{jk}(p)$ is calculation with a method described in reference [7] as follows:

$$\Delta w_{jk}(p) = \alpha \times y_j(p) \times \delta_k(p) \tag{5}$$

where α is learning rate and $\delta_k(p)$ is an error gradient defined as follows:

$$\delta_k(p) = \frac{\partial y_k(p)}{\partial X_k(p)} \times E_k(p) \tag{6}$$

In this algorithm, the sigmoid function is used for the output of the neurons. Therefore, the error gradient of Eq. (6) can be expressed as follows:

$$\delta_k(p) = \frac{\partial \left\{ \dfrac{1}{1+\mathrm{e}^{-X_k(p)}} \right\}}{\partial X_k(p)} \times E_k(p) = \frac{\mathrm{e}^{-X_k(p)}}{(1+\mathrm{e}^{-X_k(p)})^2} \times E_k(p) \tag{7}$$

Then, Eq. (6) can be re-expressed with Eq. (7) as follows:

$$\delta_k(p) = y_k(p) \times \{1 - y_k(p)\} \times E_k(p) \tag{8}$$

As a similar way, the threshold values in hidden and output layers can be calculated with the fixed value '-1' and threshold weight $\theta_k(p)$ as follows:

$$\theta_k(p+1) = \theta_k(p) + \Delta\theta_k(p) \tag{9}$$

$$\Delta\theta_k(p) = -\alpha \times \theta_k(p) \times \delta_k(p) \tag{10}$$

Based on the above equations, the algorithm of the back-propagation is pursued as follows:

i. The goal outputs in big data are normalized with maximum value '2'.
ii. All weights and threshold values are initialized with the random selections from a uniform distribution which is distributed within ($-2.4/F_i$, $+2.4/F_i$) where F_i is the number of neurons in the neural network [8].
iii. The outputs of neurons in the hidden and output layers are calculated with Eqs. (1) and (2).
iv. The error gradient of the output neuron is calculated with Eq. (8). And, the correction factors of weights and threshold values are calculated with Eqs. (5) and (10). Finally, the weights and threshold values are updated with the correction factors with Eqs. (4) and (9).
v. Steps iii and iv are repeated until sum of the errors are satisfied to the error reference.

After enough machine learnings of the ANN, the output is directly obtained with the ANN after the output is multiplied to 2 which is the maximum value set in this study. However, for the complex problems, huge initial data should be produced to confirm the accuracy of ANN. In addition, how many data is necessary to obtain an accurate result with ANN is not known. This can make a significant inefficiency problem on the use of ANN. In Section 2.2, the automatic designing method using ANN is proposed.

2.2. Optimization algorithm for reflector design with ANN

In this section, an automatic machine learning algorithm and optimization strategy of the reflector arrangement are proposed. The automatic optimization algorithm using the ANN, which was developed by C++ program language, is given as shown in Fig. 2. (Step 0) Before starting the optimization, the basic information about the previous big data and weights are updated when a big data is existed. (Step 1) When the initial big data is not existed, 100 initial data is produced with the given algorithm. The ANN can only estimate the output based on the big data. Especially, it can give a low accuracy when the big data is not enough and includes useless information. To get a better result, the ANN should be well trained with useful big data. In this study, 1 basic model, which is simply guessed by a human knowledge, was set, and the 100 initial samples are generated based on the basic model with random sampling technique. Also, the symmetric arrangement is forced to generate the sample cases. (Step 2) After the sample cases are generated, the cases are converted to MCNP inputs and (Step 3) automatically run with the MCNP6 code [9]. (Step 4) The outputs are saved into the big data for the ANN. (Step 5) The machine learning is then pursued with the big data until the sum of squared error is converged to a reference value '0.001'. Also, for the effective machine learning, the learning rate α should be properly selected. In our study, an acceleration algorithm proposed by Jacobs [10] was adopted. When the sum of squared error is exceeded with that of current iteration, the α is decreased to 0.8 times while it is increased to 1.05 times.

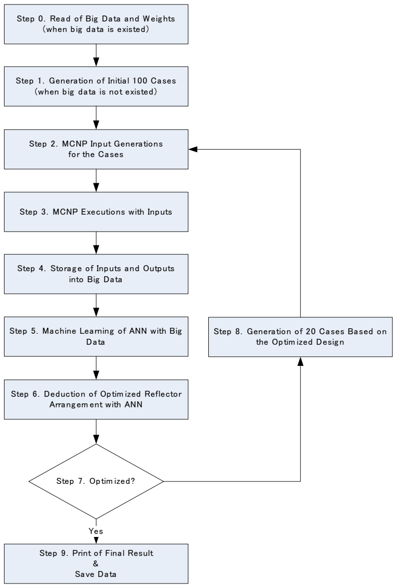


Fig. 2. Flowchart of automatic optimization algorithm for reflector design

(Step 6) After the weights and threshold values are updated from the big data, the optimized arrangement of the core components is performed using the ANN. The core (reflector) optimization is started from a model that a fuel is located at the center and the other region is filled by a basic type moderator. Using the trained ANN, the best location of the fuel, which gives a best agreement with goal output, is searched. After deciding the fuel arrangement, the positions for moderators/reflectors are searched using the ANN with the same procedure given in above. There is no way to confirm the accuracy of ANN. In this algorithm, (Step 7) the final arrangement is determined when the design is not changed after additional machine learnings were performed and updated. The additional cases are produced by the basis on the optimized arrangement determined in previous steps. First, a calculation with an optimized model pursued by previous step is performed, and (Step 8) 20 additional cases are additionally generated by locally changing the arrangement of the optimized model. The 10 samples of the 20 cases are generated by random changes of the materials maintaining the number of material fraction (fuel to non-fuel fraction). Another 10 samples are determined with exchange of the 20 material positions from the optimized model. After adding new sample cases, the estimation of Step 2 is performed. (Step 9) After determining the final design, the optimized arrangement is selected and outputs are printed.

3. Evaluation and analysis

3.1. NAA test with Problem #1

For the test of NAA, a simple problem was set as shown in Fig. 3. In the center of the sphere, U-235 fuel is located with 5 cm, and 5 reflector layers are located at out of the fuel. Each layer has 5 cm thickness, and water, graphite, beryllium, lead, and sodium were selected for the candidate materials of the reflector. The goal output was set to obtain a highest k_{eff} as the reflector arrangement. In each layer, 5 materials can be located allowing duplicate uses of the reflector materials, and therefore, 5^5 cases can be generated for the combinations of reflectors. Details on the problem are given in Table 1.

Table 1. Details on Problem #1 for the NAA test

Classification	Variable	Values
Shape	-	Sphere having 5 reflector layers
Outer radius of each region	Radius	5 cm / 10 cm / 15 cm 20 cm / 25 cm / 30 cm
Fuel	U-235 Atom Density	5.0000×10^{22} #/cm^3
Reflector	Water (H2O) Atom Density	3.3428×10^{22} #/cm^3
	Graphite Atom Density	8.6070×10^{22} #/cm^3
	Beryllium Atom Density	1.2349×10^{22} #/cm^3
	Lead Atom Density	3.2958×10^{22} #/cm^3
	Sodium Atom Density	2.5357×10^{22} #/cm^3

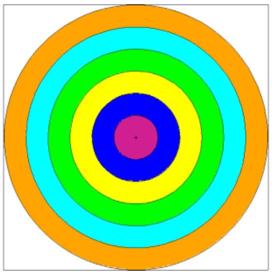


Fig. 3. Radial view of Problem #1 for NAA verification

With a uniform random sampling of the reflector, 100 sample cases were produced, and it is executed with MCNP6 code with ENDF VII.0 cross section library. After MCNP executions with the sample inputs, the ANN described in Section 2.1 was updated by the machine learning. And, the optimized arrangement was then estimated by the ANN which to achieve a highest k_{eff}. The highest k_{eff} was estimated to 1.04034 when the berylliums were selected in all reflector regions. For the verification, the MCNP calculation was pursued with the beryllium reflectors, and it was estimated to 1.05760 (±0.00141) which has a highest value among the uses of candidate reflectors. It shows that the NAA can be properly utilized for the optimization of reflector arrangement.

3.2. Test of optimization algorithm with Problem #2

To confirm that the proposed method can be utilized for the complex geometry, Problem #2 with 11 x 11 lattice structures having 5 cm x 5 cm unit lattice was set as shown in Fig. 4. Using the reflected boundary condition, infinite axial length was assumed. In the cases, following conditions are applied (the details of the material information are given in Table 2):

- 10 w/o enriched Fuel block (Number of blocks: 20)
- 20 w/o enriched Fuel block (Number of blocks: 5)
- Polyethylene block as moderator or reflector (Number of blocks: unlimited)
- Graphite block as moderator or reflector (Number of blocks: unlimited)
- Beryllium block as moderator or reflector (Number of blocks: 12)

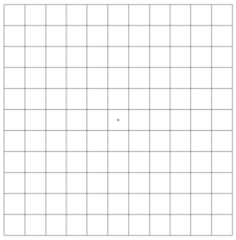
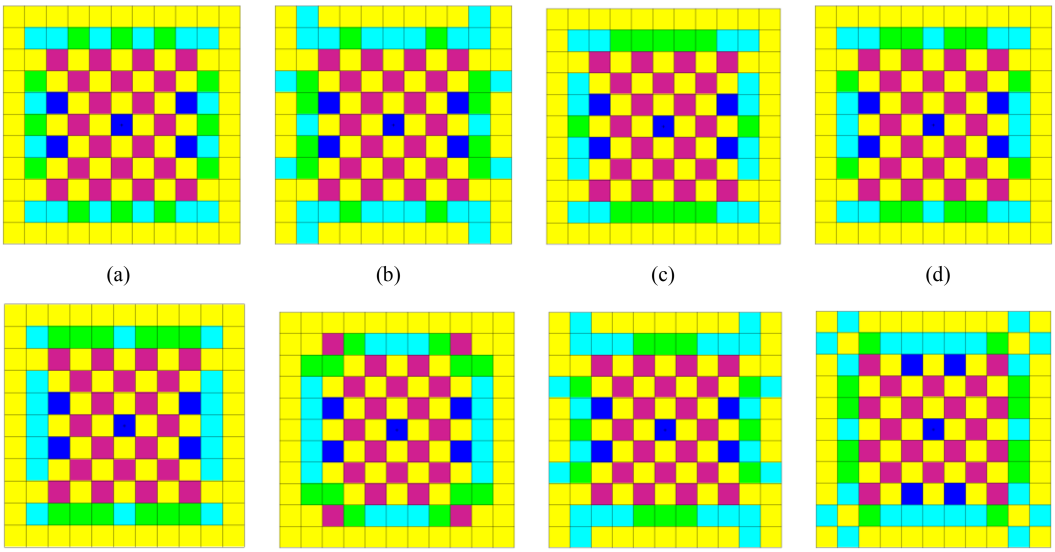


Fig. 4. Radial view of Problem #2 for verification of the proposed scheme

Table 2. Details of the core specifications on Problem #2

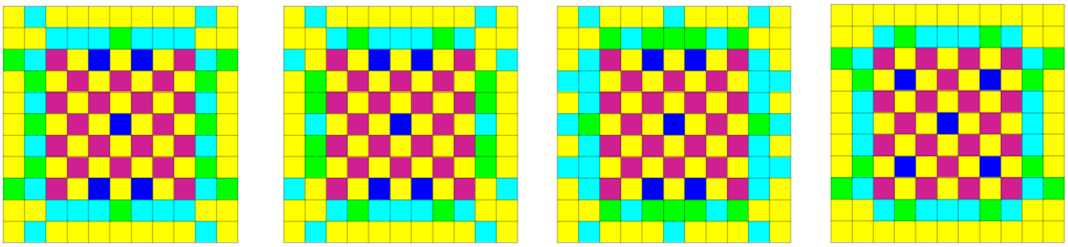
Classification	Variable	Values
Shape	-	Squire Lattice (5 cm x 5 cm)
Fuel	Density of 10 w/o enriched Fuel	5 g/cm^3
	Density of 20 w/o enriched Fuel	5 g/cm^3
Reflector	Density of Polyethylene block	0.95 g/cm^3
	Density of graphite block	1.73 g/cm^3
	Density of beryllium block	1.85 g/cm^3

With the proposed algorithm described in Section 2.2, the optimization of fuel and reflector arrangements with the given conditions was performed. All MCNP simulations and data analyses were automatically pursued with the program. The particle history for each MCNP simulation was decided to have that the uncertainties of all k_{eff} results are under the 0.001. The optimized arrangements designed by the ANN are given as shown in Fig. 5 (red: 10% enriched fuel, dark blue: 20% enriched fuel, yellow: polyethylene, green: beryllium, sky-blue: graphite). Also, the k_{eff} results calculated by the MCNP code were given in Table 3. In our analysis, these results show that the optimized designs quite approached the core design having highest k_{eff}. However, some problems with the proposed method and ANN are notified: i) uncertainty of the Monte Carlo method can cause some errors on the arrangement optimization and ii) the locations having small effect on the effective multiplication factor k_{eff} cannot be clearly determined by the ANN due to the insufficient machine learning information of the locations. In future work, it is planned that a method to resolve the problems will be developed.



(a) (b) (c) (d)

(e) (f) (g) (h)



(i) (j) (k) (l)

Fig. 5. Optimized Arrangements from the ANN and Proposed Algorithm

Table 3. Results of multiplication factors with the optimization arrangements

Arrangement	k_{eff}	Arrangement	k_{eff}	Arrangement	k_{eff}
(a)	1.24784	(e)	1.24553	(i)	1.2443
(b)	1.24406	(f)	1.23246	(j)	1.24396
(c)	1.24909	(g)	1.24567	(k)	1.24306
(d)	1.24789	(h)	1.24491	(l)	1.24352

4. Conclusion

In this study, a preliminary study for developing optimization method of the reflector arrangement was performed. An ANN program for the test study was developed by using the previous ANN theories. After constructing the ANN system using the feedforward neural network and back-propagation algorithm, an optimization algorithm for the reflector arrangements was established and programmed by C++ language. All transport calculations were performed by MCNP6 code with ENDF-VII.0 cross section library. Based on the proposed algorithm and program, the optimizations of the reflector arrangements for two problems were pursued to test the proposed algorithm. It was verified that the proposed algorithm with the ANN can be effectively and properly used for the optimization of reflector design. However, some problems on the method were notified about accuracy; uncertainty in using Monte Carlo method; and judgement selecting reflector in lowly affecting region into the output. As a future work, these problems will be resolved after developing an advanced method and algorithm.

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